

2-Nitrobutane
600-24-8 | DTXSID3020968

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.43 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.35e-01

Confidence level: 8.27e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl 2-bromoisobutyrate</div> <div>Measured: 7.79</div> <div>Predicted: 3.11</div>	<div>Image not found</div> <div>Ethyl methyl sulfide</div> <div>Measured: 6.88</div> <div>Predicted: 121</div>	<div>Image not found</div> <div>2,3-Dimethylbutan-2-ol</div> <div>Measured: 12.0</div> <div>Predicted: 5.17</div>
<div>Image not found</div> <div>Ether, isobutyl methyl</div> <div>Measured: 3.79</div> <div>Predicted: 201</div>	<div>Image not found</div> <div>Dimethylaminoethanol</div> <div>Measured: 10.1</div> <div>Predicted: 2.33</div>	